OFFICE OF NAVAL RESEARCH

GRANT N00014-95-1-1183

R&T PROJECT: pchm95d---01

PROGRAM MANAGER: Dr. P. P. Schmidt

FINAL REPORT

SIMULATIONS OF TRIBOLOGY AT CARBON/METAL INTERFACES

by

Susan B. Sinnott

The University of Kentucky
Department of Chemical & Materials Engineering
Lexington, KY

June 30, 1996

Objective:

The goal of the project is to gain an increased understanding of the atomic-scale chemical interactions responsible for macroscopic friction and wear when two surfaces are brought into sliding contact with each other. Such insight is crucial to the development of improved solid-state lubricants and, consequently, improved machines of technological and military importance. The approach is molecular dynamics simulations to provide detailed information about the tribochemistry that occurs when films of carbon solid-state lubricants, such as graphite and diamond-like carbon, are placed between two metal surfaces that are in sliding contact with each other. To facilitate realistic interactions between the covalent carbon atoms and the metal atoms, a combined many-body carbon -metal (MBCM) potential must be constructed that allows one to examine systems composed of thousands of atoms on a standard workstation.

Approach:

A combined many-body carbon-metal (MBCM) potential suitable for use in large-scale atomistic simulations has been constructed. The combined potential reduces to the reactive empirical bond order (REBO) form of Brenner et al. for carbon-carbon and carbon-hydrogen interactions, and to the corrected effective-medium (CEM) form for metal-metal interactions. The metal-carbon interactions are characterized by an expression of the effective-medium type.

Conclusions:

The MBCM potential yields results for test systems that are in good qualitative agreement with available first principles data. Most of the trends are captured correctly, and the potential could be used to study the *general* tribochemistry of a metallic material interacting with a covalently bonded material. It is also expected that the potential will open up to large scale computing many other important problems in materials and surface science, such as corrosion and heterogeneous catalysis. However, some refining will be necessary to obtain improved quantitative agreement with the first principles data and to allow charge transfer between the atoms.

Students and Postdocs funded through the grant:

At this time the PI has two students, Mr. Lifeng Qi and Mr. Matthew Flanagan. They are not supported by the grant directly. However, the grant did allow the PI to purchase most of the equipment needed for the research effort, thus allowing other funds to be used for student support.

Publications, Presentations, Patents and Reports Associated with the Grant:

None.

Transitions that Resulted from the Research:

None.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	6/28/96	Final Report 7/1/95-6/30/96

4. TITLE AND SUBTITLE
Simulations of Tribochemistry at Carbon/Metal Interfaces

5. FUNDING NUMBERS
Grant N00014-95-1-1183

6. AUTHOR(S)
Susan B. Sinnott

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
The University of Kentucky Research Foundation
Department of Chemical & Materials Engineering
177 Anderson Hall, Lexington, KY 40506-0046

8. PERFORMING ORGANIZATION REPORT NUMBER
0019893001

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Dr. P. P. Schmidt
Office of Naval Research
Ballston Tower One
800 North Quincy Street, Arlington, VA 22217-5660

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
ONR 331

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for Public Release;
Distribution Unlimited

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The goal of the project is to gain increased understanding of the atomic-scale chemical interactions responsible for macroscopic friction and wear when two surfaces are brought into sliding contact with each other. Such insight is crucial to the development of improved solid-state lubricants. The approach is molecular simulations to provide detailed information about the tribochemistry that occurs when films of carbon solid lubricants are placed between metals surfaces in sliding contact. To facilitate realistic interactions between the carbon and metal atoms, a combined many-body carbon-metal potential has beenconstr-ucted that allows for the characterize systems composed of thousands of carbon and metal atoms on a standard workstation. Testing of the potential has yielded very promising results with some room for improvment.

14. SUBJECT TERMS	15. NUMBER OF PAGES
Tribology, solid lubricants, molecular simulations	2
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	Unclassified/ Unlimited

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. 239-18
298-102